On the micromechanics of slip events in sheared, fluid-saturated fault gouge

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Abstract We used a three-dimensional discrete element method coupled with computational fluid dynamics to study the poromechanical properties of dry and fluid-saturated granular fault gouge. The granular layer was sheared under dry conditions to establish a steady state condition of stick-slip dynamic failure, and then fluid was introduced to study its effect on subsequent failure events. The fluid-saturated case showed increased stick-slip recurrence time and larger slip events compared to the dry case. Particle motion induces fluid flow with local pressure variation, which in turn leads to high particle kinetic energy during slip due to increased drag forces from fluid on particles. The presence of fluid during the stick phase of loading promotes a more stable configuration evidenced by higher particle coordination number. Our coupled fluid-particle simulations provide grain-scale information that improves understanding of slip instabilities and illuminates details of phenomenological, macroscale observations.

1. Introduction

Fault gouge is produced by wear and accumulates within the fault offset. The gouge zone evolves via brecciation of the wall rock and comminution of the constituent materials. Earthquakes occur within fault gouge and at the boundaries between gouge and wall rock; hence, it is important to understand stick-slip dynamics and the processes by which elastic energy accumulates, during the interseismic period, followed by sudden release [Brace and Byerlee, 1966; Johnson et al., 1973; Marone et al., 1990]. The dynamics of such stick-slip instabilities have been studied in laboratory experiments and in numerical simulations for dry fault gouge [Scholz et al., 1972; Marone et al., 1990; Marone, 1998a, 1998b; Mair et al., 2002; Anthony and Marone, 2005; Johnson and Jia, 2005; Mair and Hazzard, 2007; Johnson et al., 2008, 2012; Ferdowsi et al., 2013; Johnson et al., 2013; Ferdowsi, 2014; Ferdowsi et al., 2014a, 2014b, 2015].

Fluids play a significant role in altering the characteristics of stick-slip cycles; however, its role is poorly understood, and there are only a few studies in this regard [Scuderi et al., 2014, 2015a; Scuderi and Collettini, 2016]. Contact strengthening and evolution of friction are thought as the most important influences of fluids on the stick-slip dynamics of granular fault gouge. In a fully saturated granular fault gouge, researchers have studied the change of permeability [Okazaki et al., 2013; Candela et al., 2014; Scuderi et al., 2015b; Kaproth et al., 2016; Leclère et al., 2016], lubrication effect [Verberne et al., 2014], and change of fluid pore pressure and its effects [Scuderi et al., 2015a]. It is shown in experiments that the fluid pore pressure can cause triggered seismicity [Scuderi and Collettini, 2016]. Under low confining pressure, a strengthening behavior of fluid has been observed in recent experiments in submerged granular flows [Koivisto and Durian, 2017]. Progress in numerical modeling allows us to better understand the physics of granular media in grain scale [e.g., Dorostkar and Mirghasemi, 2016] and, specifically, the mechanisms at play in fluid-saturated granular fault gouge [e.g., Dorostkar et al., 2017]. Numerical modeling allows us to study the same samples in dry and saturated conditions. Moreover, we can identify the effect of granular arrangements on the stick-slip behavior and extract microscale information before and during slip event and perform parametric studies of the most important parameters. In the simulations, we can also explicitly study the mechanical (e.g., change of fluid pore pressure and fluid-particle interaction) or chemical (e.g., pressure solution and frictional healing) effects of fluids on the stick-slip behavior. An important phenomenon during stick slip of granular porous media is the occurrence of...
2. Methods

We used the discrete element method (DEM) coupled with computational fluid dynamics (CFD) and 3-D granular elements to investigate dry and fluid-saturated fault gouge (Dorostkar et al., 2017). In the DEM, the trajectory of Lagrangian solid particles is tracked by solving the equations of motion. Particle-particle interactions in the normal direction obey nonlinear Hertzian contact via the soft sphere method, which allows overlap between particles (Hertz, 1882; Di Renzo and Di Maio, 2004). The tangential force is limited by Coulomb friction.

A two-way CFD-DEM simulation procedure is applied to describe the particle-fluid interactions. We use unresolved CFD-DEM, where each CFD cell contains several particles and an interstitial fluid between grains is not considered (Goniva et al., 2012; Kloss et al., 2012). The coupling is considered by the modified Navier-Stokes equations taking into account the volume fraction occupied by particles as well as momentum exchange between particles and fluid. In addition, drag forces, pressure gradient forces, and viscous forces are summed with particle-particle interaction forces (in DEM) to incorporate the effect of the surrounding fluid on particle motion (Zhou et al., 2010). The momentum exchange includes drag forces between fluid and granular particles. We remark that we do not use lubrication forces in our CFD-DEM approach and keep the particle friction coefficient in dry and wet conditions constant. We use the Koch-Hill drag correlation appropriate for intermediate porosities as is the case in our study (Koch and Hill, 2001).

The granular layer (Figure 1) is confined in the $z$ direction with two corrugated plates, which enhance shear within the gouge layer similar to laboratory experiments and tectonic fault zones (Marone, 1998a). For gouge particles, periodic boundaries are applied in the $x$ direction and frictionless walls are used in $y$ direction. The sample size is $11 \times 1.5 \times 0.8$ mm$^3$, sufficiently large to have proper 3-D particle interactions (Ferdowsi et al., 2013; Ferdowsi, 2014). Gouge particles have a polydispersed size distribution from 45 to 75 μm, consistent with laboratory experiments that exhibit stick-slip failure (Scuderi et al., 2015a). We conducted a series of trial runs to identify the confining stress and shear velocity that result in stick-slip dynamics. Normal load condition of 10 MPa (effective stress, supported by solid particles), close to that employed in the experimental studies we are interested in simulating (Scuderi et al., 2014; Scuderi et al., 2015a), and shear velocity of 0.6 mm/s are chosen.

The description of material properties and simulation setup is given in Table 1. Gouge layers are generated by randomly adding particles of the chosen size distribution. The granular layer is then confined, and the bottom plate is moved in the $x$ direction to impose shear while holding the normal load constant.

After shearing sufficiently to develop steady state stick-slip dynamics, we introduce fluid at the onset of a stick-slip cycle everywhere in the sample at the same time with a fixed homogeneous density. The addition of fluid is a numerical procedure, and no change in position or additional force is imposed on particles. Pressure inlet/outlet boundary conditions (fixed value pressure equal to zero, nonperiodic) are considered for the left and right sides of the layer ($x$ direction). Impermeable no-slip boundary conditions are applied to the other four surfaces (top, bottom, front, and back). We use the open source software LIGGGHTS (Kloss et al., 2012) for the DEM solver, OpenFOAM (Weller et al., 1998) for the CFD calculations, and CFDEMCoUpling (Goniva et al., 2012) to couple the two models. Details of the CFD cell size, coupling interval, and stability criteria are given in the supporting information.
3. Results

Figure 2 shows representative data for the friction coefficient (Figure 2a), particle kinetic energy (Figure 2b), and relative thickness change (Figure 2d) for gouge layer sheared under dry and saturated cases. The macroscopic friction coefficient is the ratio of shear force divided by the normal force. The particle kinetic energy consists of both translational \(\frac{1}{2}m_p v_p^2\) where \(m_p\) and \(v_p\) are the particle mass and velocity) and rotational \(\frac{1}{2}I_p \omega_p^2\), where \(I_p\) and \(\omega_p\) are moment of inertia and angular velocity of particle) components summed over all particles. The relative thickness change is computed as the difference of instantaneous and average thickness (over the entire simulation time) normalized by the average thickness. Figure 2c shows the fluid kinetic energy for the saturated case (computed as \(\frac{1}{2}m_f u_f^2\) where \(m_f\) and \(u_f\) are the fluid mass and velocity).

Our simulations of stick-slip failure under dry and saturated conditions (Figure 2) show that frictional strength increases nonlinearly, reaching a maximum and then dropping suddenly during failure. During the stick phase, elastic energy is stored in the granular layer, and a portion is released as particle kinetic energy during slip, as manifested by the sharp spike in Figure 2b. During the stick phase, the granular layer dilates, whereas during failure the gouge layer compacts, i.e., a decrease in layer thickness.

The friction coefficient during the stick phase of saturated and dry cases follows a similar curve until slip. However, for saturated conditions slip event (SE\(_{sat}\)) happens later and the stress drop is larger compared to dry conditions (SE\(_{dry}\)). We also observe an increase in recurrence time of particle kinetic energy release and drop in layer thickness. The released particle kinetic energy and drop in layer thickness are larger for saturated compared to dry conditions.

From Figure 2c, we see that the occurrence of SE\(_{sat}\) is associated with an increase in fluid kinetic energy. The red inset in Figure 2c shows the fluid kinetic energy fluctuations during the stick phase due to particles

<table>
<thead>
<tr>
<th>Table 1. Simulation Properties</th>
<th>Value</th>
<th>Property</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Particle density</td>
<td>2900 kg/m(^3)</td>
<td>Particle radius</td>
<td>45–75 (\mu)m</td>
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<td>Number of particles</td>
<td>7996</td>
<td>Fluid density</td>
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<td>Particle Poisson ratio</td>
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<td>Fluid viscosity</td>
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<td>Particle Young’s modulus</td>
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<td>CFD time step</td>
<td>(10^{-7}) s</td>
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<tr>
<td>Particle friction coefficient</td>
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<td>DEM time step</td>
<td>(10^{-9}) s</td>
</tr>
<tr>
<td>Particle restitution coefficient</td>
<td>0.87</td>
<td>Coupling interval</td>
<td>(10^{-6}) s</td>
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<td>Sample size</td>
<td>11 (\times) 1.5 (\times) 0.8 mm(^3)</td>
<td>Number of CFD cell</td>
<td>1760</td>
</tr>
</tbody>
</table>
rearrangement or microslips. This inset shows that the fluid kinetic energy increases 6 to 8 orders of magnitude during the slip event. In Figure 2e, the average coordination number is shown. The coordination number is calculated in the same way for dry and saturated systems and represents number of contacts per particle (two particles are in contact if the distance between their centers is smaller than the sum of particle radii). This panel shows that introducing fluid, the coordination number increases and stays higher on average. The fluctuations in the coordination number are associated with fluid motion and particle rearrangement.

In Figure 3a and 3b, we present the distribution of particle kinetic energy over the middle portion of the specimen. This portion is found to be representative of the granular layer. The distribution shows domains with high particles kinetic energy (KE patches), both for $SE_{dry}$ and $SE_{sat}$. We observe that the KE patches for $SE_{dry}$
are more localized in the center of the specimen, while the KE patches for SE_{sat} are extended over large parts of the specimen, meaning that in the saturated case more particles are mobilized during slip. Figure 3c shows that the normalized particle-fluid interaction forces (normalized by the average value over all particles) are spread over larger zones, which are approximately coincident with the domains of high KE. Figures 3d and 3e show the fluid and particle velocity field for SE_{sat}, where the color bar represents the magnitude of velocity and the arrows show the direction of velocity vector. We observe that fluid flow during slip is characterized by high fluid velocities, which are found to be more than 2 orders of magnitude higher than the fluid velocity during the stick phase. The fluid velocity during the stick phase is around 0.06 cm/s, which is close to driving plate velocity. We remark that the average particle Reynolds number (calculated for fluid velocity with respect to particles) during the stick phase is around 0.004 and for slip events ranges between 1 and 2.
A qualitative comparison of the zones with high KE, high fluid-interaction force, and high fluid flow (Figure 3) shows that these domains are approximately coincident. This means that there is a strong correlation between the occurrence of particle movement, fluid flow, and particle-fluid interactions. We also observe in Figure 3f that the regions of high fluid flow show small changes in porosity, whereas regions of porosity increase are juxtaposed with zones of consolidation.

To better understand the origin of the particle-fluid interaction forces, we determine the drag force and pressure gradient force along the domain length averaged over the depth and height of the sample. Figure 4 shows that drag force is several orders of magnitude higher than the pressure gradient force. These high values of drag force on particles are caused by the high fluid velocities during slip as observed in Figure 3d.

4. Discussion

We observed that the presence of fluid in a granular fault gouge increases stick-slip recurrence time and results in an increase of macroscopic friction drop, particle kinetic energy, and layer compaction during stick-slip failure (Figure 2). Given that the shear velocity and the shear stress are the same in the dry and saturated cases, a longer stick phase will lead to more storage of energy, followed by a larger release of energy during slip in the saturated case. This finding is in line with our previous statistical study on a large number of slip events, where we showed that the presence of fluid increases, on average, the recurrence time between events [Dorostkar et al., 2017]. In this study, we showed that the presence of fluid in the granular layer allows rearrangement of particles reaching a more stable configuration with higher coordination number. The correlation between fluctuations in coordination number and fluid kinetic energy in fluid-saturated case witnesses this fact. Experimental observations also support our results that the fluid can stabilize the granular fault gouge and increase the recurrence time [Higashi and Sumita, 2009; Yamashita, 1999].

Another key finding is the striking increase of fluid kinetic energy and fluid velocities at slip, as seen in Figures 2c and 3d, respectively. These high fluid velocities are explained by the fact that the granular system undergoes rapid particle rearrangements at slip time, causing the fluid to move due to momentum exchange between particles and fluid. This momentum exchange is driven by drag forces between fluid and particles, as shown in Figure 4a. The high velocity of fluid flow in turn increases particle motions and their kinetic energy by drag forces, as seen in Figure 3b. The connection between these observations explains the high spatial correlation of patches of high KE, zones of high particle-fluid interactions, and fluid velocity, as shown in Figures 3b–3d, respectively. These mechanisms lead to growth of the size of the KE patches showing that a larger portion of granular layer is involved in the failure process. We note that as a result of these coupled mechanisms, also, the local porosity will change, although these changes are found to be rather small. We also mention that in our previous statistical analysis of a large number of slip events [Dorostkar et al., 2017], it was found that the drag forces between fluid and particles are the primary driving forces leading to an increase of particle kinetic energy. This was demonstrated by showing that when we turn off the drag forces, the statistical distributions of particle kinetic energy for dry and saturated cases become identical. All
these observations show the important impact of fluid flow on the characteristics of a slip event. Our findings are in agreement with experimental observations, where the role of fluid pressure was also analyzed [Scuderi et al., 2015a; Scuderi and Collettini, 2016]. In the laboratory experiments, total fluid pressure composed of both static and dynamic pressures, measured by pressure gauges, was found to increase during slip [Scuderi et al., 2015a]. Although these experiments and our simulations are not completely similar, especially regarding boundary conditions, we might hypothesize that the increase in total pressure can be attributed to the increase in dynamic pressure. We showed indeed that the dynamic pressure, also called velocity pressure, which is defined as the fluid kinetic energy per volume, will increase during slip. In our simulations, the average pore pressure is very small (50–100 Pa) during the stick phase, whereas the local dynamic pressure can reach to 5–15 kPa depending on the event size close to that of experiments with the same confining stress [Scuderi et al., 2015a].

5. Conclusions

We conducted 3-D CFD-DEM simulations for fluid-saturated granular fault gouge. We report grain-scale results of a characteristic stick-slip cycle for dry and fluid-saturated cases. Our grain-scale observations for a representative stick-slip cycle complement our macroscale observations and also are consistent with our previous statistical analysis using large number of slip events. The main findings of this research are summarized as follows:

1. The presence of fluid allows particle rearrangement reaching to a more stable configuration evidenced by higher coordination number in fluid-saturated case compared to dry case.
2. The release of particle kinetic energy during slip is higher in the saturated system, in contrast to the dry system, which is seen by more of the granular volume participating in failure process in saturated case.
3. The spatial correlation of regions with high fluid velocity, particle-fluid interaction, and particle kinetic energy during slip provides grain-scale evidence that the mechanisms of particle rearrangements, fluid velocity, and particle-fluid interaction force are strongly coupled phenomena.
4. The high velocity of flowing fluid during slip event, caused by particles rearrangement, results in an increase of drag force on particles leading in turn to a high particle kinetic energy as well as an increase in fluid dynamic pressure.

Acknowledgments

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References


Ferdowski, B. (2014), Discrete element modeling of triggered slip in faults with granular gouge: Application to dynamic earthquake triggering, PhD dissertation, ETH Zurich, Switzerland.


Introduction

Here we explain in more detail the coupled CFD-DEM method and simulation procedure. The information we provide includes details on DEM (S1), governing equations of CFD-DEM and coupling forces (S2) and CFD-DEM coupling console (S3).
**Text S1.**

**DEM:**

In DEM, the equations of motion for particles considering the force balance are solved:

\[ \sum F_{pi} = m_{pi} \left( \frac{d}{dt} u_{pi} \right), \quad (1) \]
\[ \sum T_{pi} = I_{pi} \left( \frac{d}{dt} \omega_{pi} \right), \quad (2) \]

where \( m_{pi} \), \( I_{pi} \), \( u_{pi} \) and \( \omega_{pi} \) are mass, moment of inertia, translational and angular velocity of particle \( i \), and \( F_{pi} \) and \( T_{pi} \) are forces and torques acting on particle \( i \) from particle-particle contacts, respectively. In a fluid-saturated system, we add the fluid-particle interaction as well. In DEM the contact between particles is considered by allowing particle overlap and the normal and tangential contact forces are calculated as follows [Di Renzo & Di Maio, 2004]:

\[ F_{pn} = -k_{pn} \delta \varepsilon_{pn} + c_{pn} \delta u_{pn}, \quad (3) \]
\[ F_{pt} = \min \left\{ \left[ k_{pt} \int_{t_c}^{\infty} \delta u_{pt} \, dt + c_{pt} \delta u_{pt} \right] \mu_c F_{pn} \right\}, \quad (4) \]

where \( k_{pn} \) and \( k_{pt} \) are the normal and tangential spring stiffness and \( c_{pn} \) and \( c_{pt} \) are the normal and tangential damping coefficient. In Eqs. (3) and (4), \( \delta \varepsilon_{pn} \) is the overlap and \( \delta u_{pn} \) and \( \delta u_{pt} \) are relative normal and tangential velocities of two particles in contact. The inter-particle friction coefficient that limits the tangential contact force based on the Coulomb friction law is represented by \( \mu_c \) in Eq. (4). The damping part in Eq. (4) is added to the tangential force component if the Coulomb criterion is not met. The spring and damping coefficients are calculated as follows [Di Renzo & Di Maio, 2004; Hu et al., 2010]:

\[ k_{pn} = \frac{4}{5} Y^{*} \sqrt{R^{*} \delta \varepsilon_{pn}} , \quad k_{pt} = 8 G^{*} \sqrt{R^{*} \delta \varepsilon_{pn}} , \quad (5) \]
\[ c_{pn} = -2 \frac{r}{6} \psi \sqrt{S_{n} m^{*}} , \quad c_{pt} = -2 \frac{r}{6} \psi \sqrt{S_{t} m^{*}} , \quad (6) \]
\[ S_{n} = 2 Y^{*} \sqrt{R^{*} \delta \varepsilon_{pn}} , \quad S_{t} = 8 G^{*} \sqrt{R^{*} \delta \varepsilon_{pn}} , \quad \psi = \frac{\ln(r)}{\sqrt{\ln^{2}(r)+\pi^{2}}} . \quad (7) \]

In Eq. (7), \( r \) is the restitution coefficient. In Eq. (5) to (7), \( Y^{*}, R^{*}, G^{*} \) and \( m^{*} \) are the equivalent Young’s modulus, radius, shear modulus and mass for the two particles in contact, calculated as:

\[ \frac{1}{Y^{*}} = \frac{(1-v_{1}^{2})}{y_{1}} + \frac{(1-v_{2}^{2})}{y_{2}} , \quad \frac{1}{G^{*}} = \frac{2(2-v_{1})(1+v_{1})}{y_{1}} + \frac{2(2-v_{2})(1+v_{2})}{y_{2}} , \quad (8) \]
\[
\frac{1}{k^*} = \frac{1}{k_1} + \frac{1}{k_2}, \quad \frac{1}{m^*} = \frac{1}{m_1} + \frac{1}{m_2}.
\] (9)

In Eqs. (8) and (9), subscripts 1 and 2 refer to the two particles in contact. In Eq. (8), \( \nu \) is the poison ratio of particle.

**Text S2.**

**CFD-DEM:**

In unresolved CFD-DEM, one CFD cell contains several particles meaning particles are not resolved but their interaction with the fluid is considered. The size of CFD cell in our simulations is selected based on a sensitivity analysis. The CFD cell should be small enough to give accurate results. However, the CFD cell should also contain appropriate number of particles due to averaging-based nature of unresolved CFD-DEM method. In CFD-DEM, the modified Navier-Stokes equations of fluid mass and momentum conservation are considered. These modified equations consider the fluid volume fraction due to presence of particles and the momentum source owing to particle motion. Therefore, a two way coupling between the particle system and the fluid system is achieved. Equations (10) and (11) show the fluid mass and momentum conservation in CFD-DEM [Zhou et al., 2010]:

\[
\frac{\partial (\varepsilon_f)}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u}) = 0
\] (10)

\[
\frac{\partial (\rho_f \varepsilon_f \mathbf{u})}{\partial t} + \nabla \cdot (\rho_f \varepsilon_f \mathbf{u} \mathbf{u}) = -\varepsilon_f \nabla p + F_{pf} + \varepsilon_f \nabla \cdot \mathbf{\tau},
\] (11)

where \( \varepsilon_f \) is the fluid volume fraction, \( \rho_f \) is the fluid density (constant for the incompressible fluid), \( \mathbf{u} \) is the fluid velocity, \( p \) is the fluid pressure and \( \mathbf{\tau} \) is the shear stress tensor of fluid. In Eq. (11), the momentum exchange between particles and fluid is shown by \( F_{pf} \). This momentum exchange term is calculated for each fluid cell and is based on particle drag force. The momentum exchange between particle and fluid is calculated as follows:

\[
F_{pf} = \frac{1}{\Delta V} \sum_{i=1}^{n} (f_{p,f})_i,
\] (12)

where \( (f_{p,f})_i \) is the drag force on particle \( i \) from the surrounding fluid having \( n \) particles in the CFD cell and \( \Delta V \) being the CFD cell volume. The drag force is calculated as [Koch & Hill, 2001]:

\[
\text{drag force} = \frac{1}{8} \frac{C_d \rho_f \mathbf{u}^2}{\varepsilon_f},
\]
The drag force given by Koch and Sangani is determined using the following equation:

\[ f_{pf} = \frac{V_p \beta}{a_p} (u_f - u_p), \]  

(13)

where \( \beta = \frac{18\mu_f (1-\alpha_f)^2 \alpha_p^2}{a_p^2} (F_0(\alpha_p) + \frac{1}{2} F_3(\alpha_p)Re_p), \) \( i \) (14)

and for \( \alpha_p = 1 - \alpha_f \) and \( Re_p = \frac{\alpha_f \rho_f |u_f - u_p| d_p}{\mu_f} \). In Eqs. (13) and (14), \( f_{pf} \) is the drag force between particle and fluid, \( V_p \) is the particle volume, \( u_f \) and \( u_p \) are fluid and particle velocity, \( \mu_f \) is the fluid viscosity and \( \rho_f \) is the fluid density, \( d_p \) is diameter of particle, \( \alpha_p \) is the volume fraction of CFD cell occupied by particle and \( \alpha_f \) is the volume fraction occupied by the fluid. The function \( F_0(\alpha_p) \), that is the non-dimensional Stokes-flow drag force given by Koch and Sangani, is defined as \([Koch & Sangani, 1999; Koch & Hill, 2001]\):

for \( \alpha_p < 0.4 : F_0(\alpha_p) = \frac{1 + 3 \left( \frac{\alpha_p}{2} + (135/64) \alpha_p ln(\alpha_p) + 16.14 \alpha_p^2 \right)}{1 + 0.681 \alpha_p - 8.48 \alpha_p^2 + 8.16 \alpha_p^3}, \) \( i \) (15)

and for \( \alpha_p > 0.4 : F_0(\alpha_p) = \frac{10 \alpha_p}{(1-\alpha_p)^3} \) \( i \) (16)

and further: \( F_3(\alpha_p) = 0.0673 + 0.212 \alpha_p + \frac{0.0232}{(1-\alpha_p)^3} \) \( i \) (17)

For particle-fluid interaction in DEM model, the drag force is considered in addition to the force related to pressure gradient and the viscous force. These forces are determined as:

\[ f_p^p = -V_p \nabla p, \]  

(18)

\[ f_p^v = -V_p \nabla \tau, \]  

(19)

where \( V_p \) is the particle volume, \( p \) is fluid pressure and \( \tau \) is the shear stress tensor of the fluid.

**Text S3.**

**CFD-DEM Coupling console:**

In the two-way coupling approach of CFD-DEM method, the CFD and DEM solvers sequentially solve the governing equations and a coupling console transfers data and exchanges resultant forces between the two solvers \([Goniva et al., 2012; Kloss et al., 2012]\). First, the DEM solver calculates the particles positions and velocities by solving equation of motion (Eqs. (1) and (2)). Then the coupling console transfers particle data to the CFD solver. An Euler–Lagrange mapping algorithm finds the corresponding cell in the CFD domain for each particle. In our simulations the so-called
“divided” particle-mapping algorithm is employed that can smooth the exchange fields. Thereafter, the particle volume fraction and a mean particle velocity is calculated for each CFD cell. The fluid-particle interaction forces from surrounding fluid on each particle are calculated. The particle-momentum exchange term is calculated from particle-based forces doing an ensemble averaging over all particles in each cell. Afterward, the fluid forces acting on each particle are transferred to the DEM solver. The CFD solver calculates the fluid velocity by solving the modified Navier-Stokes equations (Eqs. (10) and (11)). These steps are repeated for every time step. During the calculations, the Courant–Friedrichs–Lewy number is continuously monitored to ensure it remains within an acceptable range of less than 1, which assures the stability of CFD calculations [Anderson & Wendt, 1995]. This criterion is related to the CFD cell size and time step. A sensitivity analysis is done for a large number of slip events in order to guarantee the independency of results to the coupling interval that the coupling console uses for transferring information between DEM and CFD solvers.

References